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14. ABSTRACT
This collaborative research has developed rigorous mathematical and computational frameworks for ROM generation and the use of ROMs in real-time, design, control, and probabilistic applications of relevance to the Air Force. This research has provided theoretical analyses and numerical studies for several new/extensions of existing ROM approaches, such as a goal-oriented, model-constrained approach, balanced truncation model reduction (BTMR) of descriptor systems, and the integratio of domain decomposition and BTMR for systems with localized nonlinearities. Additionally, several important questions related to the design, analysis, efficient computation, and application of ROM were studied. The use of ROMs was demonstrated on example applications, including optimal flow control of linearized Navier-Stokes equations, linearized flow control of a supersonic diffuser, subsonic compressor blade row unsteady aerodynamics and geometric mistuning, a thermal design problem, and nonlinear combustor model dynamics.

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COLLABORATIVE RESEARCH: AN OPTIMIZATION FRAMEWORK BASED ON DOMAIN DECOMPOSITION AND MODEL REDUCTION

FA9550-06-1-0245, FA9550-06-0271

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Abstract

Reduced order modeling (ROM) seeks to systematically extract the important dynamics from a high fidelity, high dimensional dynamical system such that outputs of interest generated by the high fidelity simulation and the ROM over a range of input parameters are within user-specified bounds. ROM is important in real-time applications, design, control, and probabilistic analyses, where outputs of interest need to be evaluated quickly for various input parameters.

This collaborative research has developed rigorous mathematical and computational frameworks for ROM generation and the use of ROMs in real-time, design, control, and probabilistic applications of relevance to the Air Force. This research has provided theoretical analyses and numerical studies for several new/extensions of existing ROM approaches, such as a goal-oriented, model-constrained approach, balanced truncation model reduction (BTMR) of descriptor systems, and the integration of domain decomposition and BTMR for systems with localized nonlinearities. Additionally, several important questions related to the design, analysis, efficient computation, and application of ROM were studied. The use of ROMs was demonstrated on example applications, including optimal flow control of linearized Navier-Stokes equations, linearized flow control of a supersonic diffuser, subsonic compressor blade row unsteady aerodynamics and geometric mistuning, a thermal design problem, and nonlinear combustor model dynamics.

1   Introduction

With the advent of efficient algorithms and high performance computers, the use of high-fidelity numerical simulations of fluid systems is moving from single-run calculations that explore flow physics towards multi-run engineering optimization calculations and probabilistic analyses. These studies require the repeated numerical simulation of a complex system to determine outputs of interest for varying design/control/input parameters.

Reduced order modeling seeks to systematically extract the important dynamics from a high fidelity dynamical system, involving a huge number of degrees of freedom, in such a way that the error between outputs of interest generated by the costly high fidelity simulation and the inexpensive low dimensional reduced order model (ROM) over a range of input parameters is below a user-specified tolerance.

Although there has been gratifying progress in design and analysis of ROM methods (see, e.g., [3]) and the application of ROM to aerospace systems (see e.g., [16]), the design of ROM approaches, derivation of error bounds, and the efficient computational implementation of ROM approaches for systems with relevance to Air Force applications pose many challenges. This collaborative research has successfully tackled several important theoretical and algorithmic issues related to the design, analysis, and efficient computation of ROM for problem classes which are important in Air Force applications. Furthermore, the use of ROMs was demonstrated on several example applications with relevance to the Air Force, including optimal flow control of linearized Navier-Stokes equations, linearized flow control of a supersonic diffuser, subsonic compressor blade row unsteady aerodynamics and geometric mistuning, a thermal design problem, and nonlinear combustor model dynamics. The techniques developed in this research have also been applied to reduced order modeling of nonlinear systems arising in the computational simulation of large neuron systems.

2   Accomplishments

This project has considered projection based model reduction methods. Abstractly the original system (typically a discretized system of partial differential equations) can be written as

$$\dot{y}(t) = f(y(t), u, t) \qquad\qquad t \in (0, T), \qquad\qquad (1a)$$
$$z(t) = g(y(t), u, t) \qquad\qquad t \in (0, T), \qquad\qquad (1b)$$

where $y(t) \in \mathbb{R}^N$ is the system state ($y(t)$ are, for example, velocities and pressure at time t), u are the possibly time dependent inputs (design variables, controls, uncertain system parameters), and $z(t) \in \mathbb{R}^k$ are the outputs of interest. We seek a reduced order model of he form

$$\dot{\hat{y}}(t) = \mathcal{W}^T f(\mathcal{V}\hat{y}(t), u, t) \qquad\qquad t \in (0, T), \qquad\qquad (2a)$$
$$\hat{z}(t) = g(\mathcal{V}\hat{y}(t)(t), u, t) \qquad\qquad t \in (0, T), \qquad\qquad (2b)$$

where $\hat{y}(t) \in \mathbb{R}^n$ is the reduced system state, $n \ll N$. As before, u are the inputs and $\hat{z}(t) \in \mathbb{R}^k$ are the outputs of interest, which are now generated via a reduced state equation (2a). The matrices $\mathcal{V}, \mathcal{W} \in \mathbb{R}^{N \times n}$ satisfy $\mathcal{W}^T \mathcal{V} = I$.

This research has addressed several important questions related to the computation of the projection matrices $\mathcal{V}, \mathcal{W} \in \mathbb{R}^{N \times n}$, estimates for the error $\|z - \hat{z}\|$ between outputs of the full and the reduced order model, and fast computation of reduced order models for nonlinear models. Specifically, this research investigated a goal-oriented, model-constrained approach, balanced truncation model reduction (BTMR) of descriptor systems, and the integration of domain decomposition and BTMR for systems with localized nonlinearities. Several important questions related to the design, analysis, efficient computation, and application of ROM in the context of applications of relevance to Air Force were studied.

Furthermore, the use of ROMs was demonstrated on several test problems which are relevant for Air Force applications, including optimal flow control of linearized Navier-Stokes equations, linearized flow control of a supersonic diffuser, subsonic compressor blade row unsteady aerodynamics and geometric mistuning, a thermal design problem, and nonlinear combustor model dynamics. The techniques developed in this research have also been applied to reduced order modeling of nonlinear systems arising in the computational simulation of large neuron systems.

The findings of this research are described below. Additional details and references may be found in the papers [2, 5, 6, 7, 8, 12, 13, 14, 15, 18, 19] and theses [4, 9, 10, 17].

2.1 Balanced Truncation Model Reduction for the Linearized Navier-Stokes Equations

Balanced Truncation Model Reduction (BTMR) is a particular model reduction method that preserves asymptotic stability and also provides an error bound on the discrepancy between the outputs of the full and reduced order system. Unfortunately, the vast majority of papers on BTMR apply this technique to dynamical systems of ordinary differential equations, but are not directly applicable to dynamical systems governed by incompressible flows, which lead to large-scale system of differential algebraic equations.
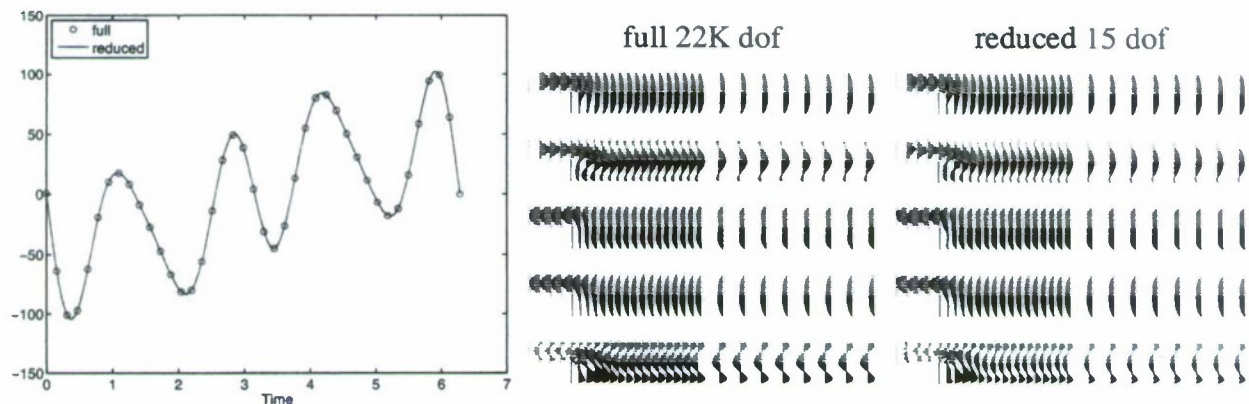

Figure 1: Left plot: Time response for the full order model (circles) and for the reduced order model (solid line). Right plot: Velocities generated with the 22K dof full order model (left column) and with the 15 dof reduced order model (right column) at $t = 1, 3, 4, 5, 6$ (top to bottom).

The work [12, 17] describes an extention of BTMR to a class of differential algebraic dynamical

systems including, e.g., linearized Navier-Stokes equations, linearized around steady flow. The procedure in [12, 17] can serve as a template for handling numerous other similar problems arising from CFD. The major advantages of this approach are that it operates on the original equations and not the projected ones, that it considerably reduces storage requirements, and that it utilizes more straightforward linear algebra techniques based upon saddle point solvers that are most likely already available to a user. Finally, the approach in [12, 17] produces reduced order models with guaranteed error bounds.

To illustrate the last point, the linearized Navier-Stokes equations in a backward facing step domain is considered. The inputs are suction/blowing controls applied on the inflow and backward facing step boundary, the output of interest is the integrated vorticity in the region behind the backward facing step. Figure 1 shows an excellent agreement between the time response of the full order model and of the reduced order model for an arbitrary input. This excellent agreement is a consequence of the theoretical error bound between the original and reduced order model. The right plot Figure 1 shows the velocity profiles generated by the original and the reduced order system. There are slight differences, but these are to be expected since the balanced reduction was designed generate a reduced order model that faithfully reproduces the integral of vorticity.

2.2 Numerical Solution of Large Scale Lyapunov Equations Using Inexact Linear System Solves

A computationally expensive part of BTMR is the computation of approximate controllability and observability Gramians. If one computes them as approximate solutions of the controllability and observability Lyapunov equations via iterative methods, such as the multishift ADI Algorithm, then in each iteration one has to solve large scale linear systems resulting from PDE discretizations. For very large scale problems, especially 3D problems, these systems have to be solved iteratively. The thesis [17] gives a detailed analysis of the impact of these iterative, hence inexact linear system solves on the convergence of the ADI Algorithm as well as on the quality of the computed solution. Inexact linear system solves have little impact on the convergence behavior as well as on the quality of the computed solution, provided the stopping criteria for the linear system solves are sufficiently fine relative to the ADI convergence rate and stopping tolerance.

2.3 Coupling with Local Nonlinearities

BTMR is one of the very few model reduction techniques for which error bounds between the input-output map of the full and reduced order model are available. Unfortunately, these are only available for linear time invariant systems. In this research we have extended BTMR to systems with spatially localized nonlinearities [17, 18]. Domain decomposition techniques are used to divide the problem into linear subproblems and small nonlinear subproblems. It also identifies interface conditions between the linear and the nonlinear subdomains. BTMR is applied to the linear subproblems with inputs and outputs determined by the original in- and outputs as well as the interface conditions between the subproblems. Figure 2 shows the result of our approach for a PDE that couples the nonlinear Burgers equation on $[-1, 1]$ to the heat equation on $[-10, -1]$,

[1, 10]. The linear parts are reduced and joined with the nonlinear Burgers equation. The plots show an excellent agreement between full and reduced order models.
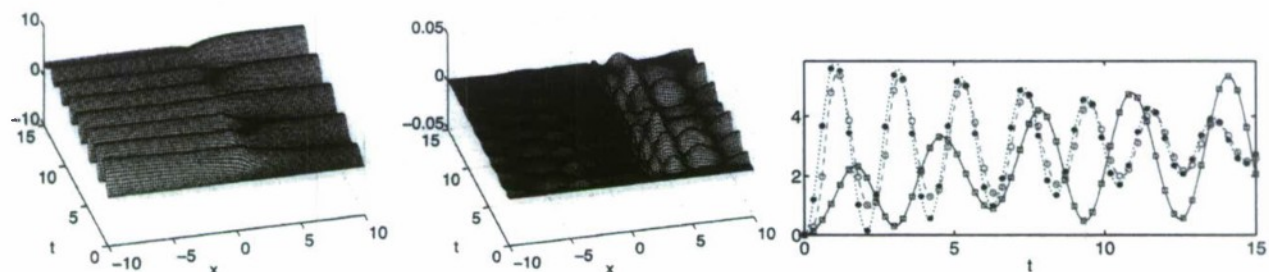

Figure 2: Left: Solution of the reduced order discretized PDE. Center: Error between the solution of the discretized PDE and the reduced order system. Right: Outputs 1, 2, 3 of the full order system are given by *, ○ and □. Outputs 1, 2, 3 of the reduced order system are given by dotted, dashed and solid lines.

The thesis contains [17] contains additional results for other test problems.

2.4 Model Reduction for Large-Scale Systems with High-Dimensional Parametric Input Space

The computation of projection matrices $\mathcal{V}, \mathcal{W} \in \mathbb{R}^{N \times n}$, such that the error $\|z - \hat{z}\|$ between outputs of the full and the reduced order model is minimized over a range of system inputs u can be viewed as an optimization problem. The approximate solution of this optimization problem is very challenging, especially for parametric input spaces of high dimension. We have proposed a model-constrained adaptive sampling methodology for reduction of large-scale systems with high-dimensional parametric input spaces. Our model reduction method uses a reduced basis approach, which requires the computation of high-fidelity solutions at a number of sample points throughout the parametric input space. The papers [4, 8] pose the task of determining appropriate sample points as a partial differential equation (PDE) - constrained optimization problem, which is implemented using an efficient adaptive algorithm that scales well to systems with a large number of parameters. For a heat transfer optimal design application with 18,000 states, the approach is demonstrated for parametric input spaces up to dimension 21 (see [8]). Sampling such high-dimensional input spaces with statistically-based sampling methods is, in general, a computationally prohibitive proposition; the model-constrained sampling developed as part of this research yields reduced models with errors three to four orders of magnitude lower than those obtained using standard methods, such as Latin hypercube and log-random sampling.

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	CFD	Reduced
Model size	103,008	201
Offline cost	–	2.8 hours
Online	501.1 hours	0.21 hours
Blade 1 mean	-1.8572	-1.8573
Blade 1 variance	2.687e-4	2.682e-4
Blade 2 mean	-1.8581	-1.8580
Blade 2 variance	2.797e-4	2.799e-4

Table 1: Linearized CFD model and reduced-order model MCS results. Work per cycle is predicted for blade plunging motion at an interblade phase angle of 180° for 10,000 randomly selected blade geometries.

The method has been applied to derive efficient reduced-order models for probabilistic analysis of the effects of blade geometry variation for a two-dimensional model problem governed by the Euler equations [5, 6]. The CFD model uses a discontinuous Galerkin formulation, and has 51,504 states per blade passage. Figure 3 shows the results of a Monte Carlo simulation (MCS) to analyze the impact of blade geometry variabilities on the work per cycle (WPC), which is defined as the integral of blade motion times the lift force over one unsteady cycle. The case shown considers two blades moving in plunging motion with an interblade phase angle of 180°. The same 10,000 geometries were analyzed using the CFD model and a reduced model of dimension 201. Figure 3 shows the resulting probability density functions of WPC for the first blade. Table 1 shows that the CPU time required to compute the reduced model MCS is a factor of more than 2000 times smaller than that required for the CFD MCS. Table 1 also compares the statistics of the two distributions. It can be seen that the reduced-order model predicts the mean, variance and shape of the distribution of WPC accurately. To further verify the quality of the reduced model, the Kolmogorov-Smirnov method is applied to test whether the reduced WPC results and the full WPC results are drawn from a same distribution. The results show that the hypothesis that the distribution is the same at a 5% significance level cannot be rejected.

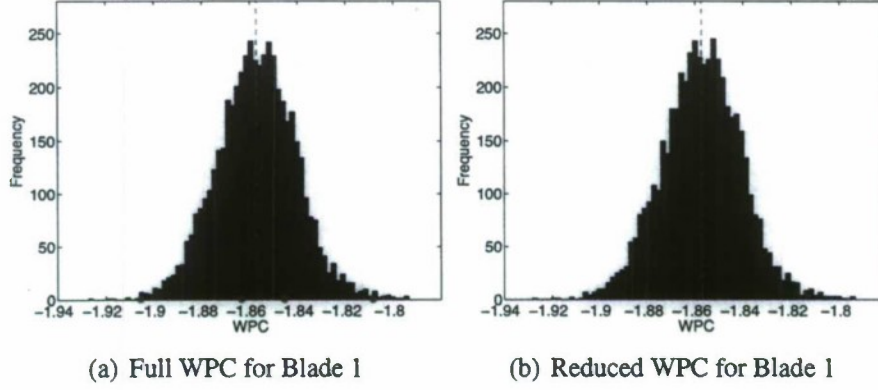(a) Full WPC for Blade 1   (b) Reduced WPC for Blade 1

Figure 3: Comparison of linearized CFD and reduced-order model predictions of WPC for Blade 1. MCS results are shown for 10,000 blade geometries. The same geometries were analyzed in each case.

2.5 Efficient Evaluation of Projection Based Reduced Order Models for Nonlinear Systems

Methods such as the proper orthogonal decomposition (POD) and the optimization-based approach [5, 6]. can be used to compute a reduced basis $\mathcal{V} = \mathcal{W}$ for nonlinear systems; however, naive projection of the governing equations onto the reduced basis can lead to a reduced model that has a small number of states but is computationally expensive to solve, since evaluation of the nonlinear term

$$\underbrace{\widehat{y}(t)}_{\in \mathbb{R}^n} \mapsto \underbrace{\mathcal{V}\widehat{y}(t)}_{\in \mathbb{R}^N} \mapsto \underbrace{f(\mathcal{V}\widehat{y}(t), u, t)}_{\in \mathbb{R}^N} \mapsto \underbrace{\mathcal{V}^T f(\mathcal{V}\widehat{y}(t), u, t)}_{\in \mathbb{R}^n}$$

will in general require computations on the large scale ($\mathbb{R}^N$).

This research has combined the model-constrained sampling algorithm described in Section 2.4 with the Empirical Interpolation Method of [1, 11] for efficient representation of nonlinearities. In this approach, the nonlinearities are represented using a coefficient-function approximation that enables the development of an efficient offline-online computational procedure where the online computational cost is independent of the size of the original large-scale model.
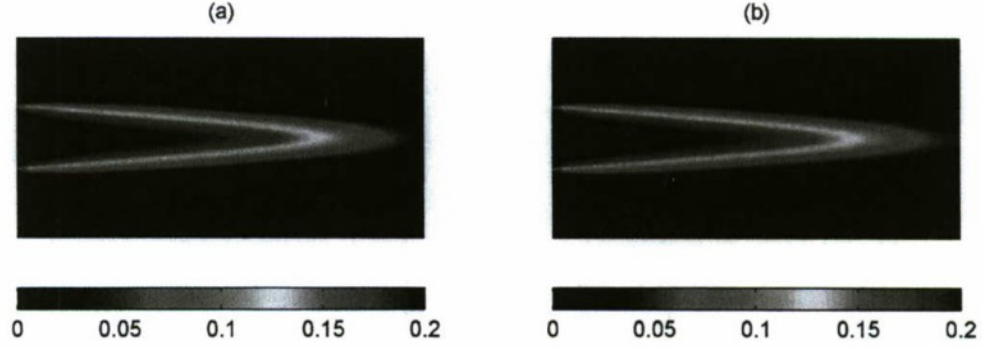
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Figure 4: Comparison of (a) finite element solution and (b) reconstructed solution using the efficient reduced basis approximation for nonlinear convection-diffusion-reaction problem.

The nonlinear model reduction methodology was applied to a highly nonlinear combustion problem governed by a convection-diffusion-reaction PDE [10]. The reduced basis approximation developed for this problem is up to $50,000$ times faster to solve than the original high-fidelity finite element model with an average relative error in prediction of outputs of interest of $2.5 \cdot 10^{-6}$ over the input parameter space. Figure 4 shows a sample comparison between the solution field computed using the efficient reduced basis approximation and the truth finite element solution for a random point in the parameter space. The reconstructed field is virtually indistinguishable from the original finite element solution.

Additionally, an alternative view of the Empirical Interpolation Method was developed in [9]. It is applicable to fully discretized systems and uses matrix-vector representations of the discretized system, rather than the variational form of the PDE and Galerkin discretization. The presentation in [9] also provides alternative error bounds for EIM based on matrix analysis.

Additionally, the nonlinear model reduction based on POD and EIM was applied to a nonlinear system arising in the computational modeling of neuron systems. In the first example the voltage in a neuron was modeled using the highly nonlinear Hodgkin-Huxley model. The neuron receives pulses from three branches. The output of interest is the voltage at a node in the neuron. Figure 5 shows an excellent agreement between the full order model with roughly N=1200 degrees of freedom and the reduced order mode with $n = 30$ degrees of freedom. The application of the reduced order model is about 10 times faster than the application of the full order model. The spiking behavior of the voltage in the neuron is captured by the reduced order model.
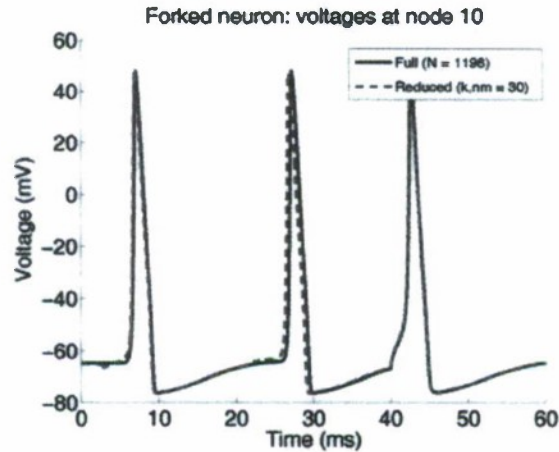
Figure 5: Full and reduced order modeling of the voltage in a neuron modeled by the nonlinear Hodgkin-Huxley equations. The spiking behavior is captured by the reduced order model, which can be executed 100 times faster than the full order model.

Another test uses the FitzHough-Nagumo equations to model a neuron. Figure 6 shows that the reduced order model can capture the limit cycle behavior of the original full order model.
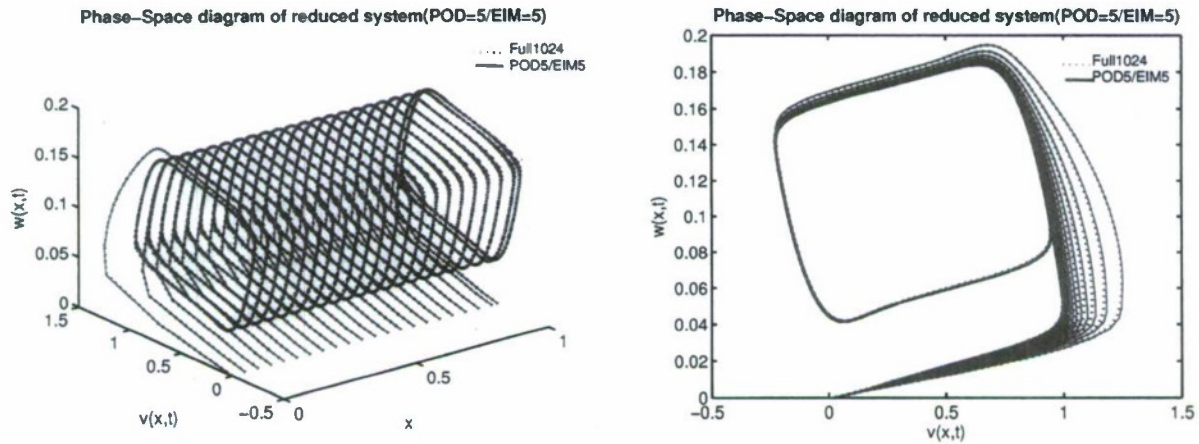

Figure 6: Full and reduced order model of the FitzHough-Nagumo equations. The reduced order model captures the limit cycle behavior of the original full order model.

Acknowledgment/Disclaimer

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